

# Feshbach resonances in ultracold ${}^6,{}^7\text{Li} + {}^{23}\text{Na}$ atomic mixtures

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(Dated: June 6, 2008)

We report a theoretical study of Feshbach resonances in  ${}^6\text{Li} + {}^{23}\text{Na}$  and  ${}^7\text{Li} + {}^{23}\text{Na}$  mixtures at ultracold temperatures using new accurate interaction potentials in a full quantum coupled-channel calculation. Feshbach resonances for  $l = 0$  in the initial collisional open channel  ${}^6\text{Li}(f = 1/2, m_f = 1/2) + {}^{23}\text{Na}(f = 1, m_f = 1)$  are found to agree with previous measurements, leading to precise values of the singlet and triplet scattering lengths for the  ${}^6,{}^7\text{Li} + {}^{23}\text{Na}$  pairs. We also predict additional Feshbach resonances within experimentally attainable magnetic fields for other collision channels.

PACS numbers:

A Feshbach resonance occurs when the kinetic energy of two colliding atoms matches the energy of a bound level associated with a closed channel [1]. Since the first experimental observation in a Bose-Einstein condensate (BEC) of sodium [2], Feshbach resonances have been widely used as a tool for controlling interactions in ultracold atomic gases. One can vary the sign and strength of the interactions by tuning the magnetic field near such a resonance, allowing the study of ultracold atomic gases from the strong interacting to the non-interacting regime [3]. For instance, BECs of  ${}^{133}\text{Cs}$  [4] or  ${}^{85}\text{Rb}$  [5] have been realized using this technique to reverse the sign of the scattering length from negative to positive. Furthermore, Feshbach resonances can be used as a spectroscopic tool [6], and provide a way of making ultracold molecules [7]. They allow for the coherent coupling between atomic and molecular condensates [8], as well as the creation of molecular BECs [9]. More details can be found in Ref. [10]

Recently, Feshbach resonances have been observed in Bose-Fermi mixtures of  ${}^6\text{Li}$  and  ${}^{23}\text{Na}$  [11] as well as in  ${}^{87}\text{Rb}$  and  ${}^{40}\text{K}$  [12], opening the door to new phenomena such as boson-mediated Cooper pairing [13] or the formation of heteronuclear molecules [14]. Such polar molecules may have applications in quantum computation [15], as well as in the search for the electronic dipole moment [16], or study of degenerate gases with dipolar interactions [17]. The most common theoretical treatment of cold collisions is the coupled-channel calculation approach [18], although several simplified methods have been developed [19]. These techniques were applied to K-Rb mixtures by Simoni *et al.* [20] and to mixed-isotope mixtures of rubidium by Burke *et al.* [21].

In this article we present an extensive theoretical study of the scattering properties of  ${}^6,{}^7\text{Li}$  and  ${}^{23}\text{Na}$  in the presence of a magnetic field and at the temperature range typical of degenerate gases (i.e. between 300 nK and 1  $\mu\text{K}$ ). Since Li has both fermionic and bosonic isotopes, Li-Na mixtures are of particular interest. We focus our efforts on finding the positions and widths of Feshbach resonances for various collision channels. This information will be useful for future experiments on cold Li-Na

mixtures, *e.g.* to form a BEC of polar molecules.

For two alkali atoms of relative momentum  $\vec{p}$  and reduced mass  $\mu$  colliding in a magnetic field, the effective two-body Hamiltonian can be written as [22]

$$H = \frac{p^2}{2\mu} + \sum_{j=1}^2 H_j^{\text{int}} + V^c + V^d, \quad (1)$$

where  $H_j^{\text{int}}$  is the internal energy of atom  $j$ ,  $V^c$  the Coulomb interaction, and  $V^d$  the magnetic dipole-dipole interaction (often neglected [10]).  $H_j^{\text{int}}$  consists of the hyperfine and Zeeman contributions, respectively

$$H_j^{\text{int}} = \frac{a_{\text{hf}}^{(j)}}{\hbar^2} \vec{s}_j \cdot \vec{i}_j + (\gamma_e \vec{s}_j - \gamma_n \vec{i}_j) \cdot \vec{B}. \quad (2)$$

Here  $\vec{s}_j$  and  $\vec{i}_j$  are the electronic and nuclear spin of atom  $j$ ,  $a_{\text{hf}}^{(j)}$  its hyperfine constant (152.1368407 MHz for  ${}^6\text{Li}$ , 401.752 MHz for  ${}^7\text{Li}$  and 885.813 MHz for  ${}^{23}\text{Na}$ ), and  $\vec{B}$  is the external magnetic field assumed in the  $z$ -direction.

The Coulomb interaction, which depends only on the internuclear separation  $R$ , can be decomposed into singlet and triplet contributions

$$V^c = V_0(R)P^0 + V_1(R)P^1, \quad (3)$$

where  $V_0$  ( $V_1$ ) and  $P^0$  ( $P^1$ ) stands for the singlet (triplet) molecular potential and its associated projection operator respectively [1]. Molecular potentials were constructed by smoothly connecting the inner part to the long-range dispersion expansion

$$V_{\text{LR}} = -\frac{C_6}{R^6} - \frac{C_8}{R^8} - \frac{C_{10}}{R^{10}} \pm C_{\text{ex}} e^{-bR} \quad (4)$$

where  $\pm$  are for the triplet and singlet potential respectively. We used the singlet potential of Fellows [23], constructed from accurate spectroscopic data via the inverse perturbation approach (IPA), and an *ab initio* triplet potential computed using the *CIPSI* package [24] and adjusted to match the atomic dissociation energy of  $\text{Li}(2s) + \text{Na}(3s)$  at infinity. For the long range form of both potentials, we adopted the dispersion coefficients ( $C_n$  and exchange energy ( $C_{\text{ex}}$  and  $b$ ) of Fellows (case a) [23].

At ultracold temperatures,  $s$ -wave collisions describe the scattering process. The collision entrance channel is determined by the initial Zeeman states of the atoms. A judicious choice of basis is the field dressed molecular hyperfine states [18]:  $|\alpha\beta\rangle$ , with  $\alpha = 1, \dots, 6$  for  ${}^6\text{Li}$ ,  $\alpha = 1, \dots, 8$  for  ${}^7\text{Li}$ , and  $\beta = 1, \dots, 8$  for  ${}^{23}\text{Na}$ , all in the increasing order of energy. We follow this standard labeling throughout the article. In the limit  $B = 0$ , it reduces to the product of atomic hyperfine states

$$|f_1, m_1; f_2, m_2\rangle \equiv |f_1, m_1\rangle_{\text{Li}} \otimes |f_2, m_2\rangle_{\text{Na}} \quad (5)$$

where  $\vec{f}_j = \vec{s}_j + \vec{i}_j$  is the total spin of atom  $j$ , and  $m_j$  its projection onto the molecular axis. This basis is suitable for description of the collision in the limit of two separated atoms. At smaller separation, the molecular basis  $|SIFM_F\rangle$  becomes more appropriate, with  $\vec{S} = \vec{s}_1 + \vec{s}_2$ ,  $\vec{I} = \vec{i}_1 + \vec{i}_2$ ,  $\vec{F} = \vec{f}_1 + \vec{f}_2$ , and  $M_F$  its projection.

Once the bases are defined, one can express Eq.(1) in matrix form, leading to the following matrix equation

$$\frac{d^2}{dR^2} \mathbf{F}(R) = \frac{2\mu}{\hbar^2} \mathbf{M}(R) \mathbf{F}(R), \quad (6)$$

where the coupling matrix  $\mathbf{M}(R)$  is defined as

$$\mathbf{M}_{(\alpha,\beta)}^{(\alpha',\beta')}(R) \frac{\delta(R-R')}{RR'} = \langle R(\alpha,\beta) | V^c | R'(\alpha',\beta') \rangle, \quad (7)$$

and  $\mathbf{F}(R)$  is a matrix with columns corresponding to a complete set of linearly independent solutions.

To obtain results with the level of accuracy given in the experimental measurements of Stan *et al.* [11], we needed to include the nuclear Zeeman term  $\gamma_n \vec{i}_j \cdot \vec{B}$  and the magnetic dipole-dipole interaction term  $V^d$  [25]. The latter one can be written as

$$\begin{aligned} V^d &= -\alpha_{\text{fs}}^2 \frac{3(\hat{\mathbf{R}} \cdot \hat{\mathbf{s}}_1)(\hat{\mathbf{R}} \cdot \hat{\mathbf{s}}_2) - \hat{\mathbf{s}}_1 \cdot \hat{\mathbf{s}}_2}{R^3} \\ &= -\frac{\alpha_{\text{fs}}^2 \sqrt{6}}{R^3} \sum_{q=-2}^2 (-1)^q C_q^2(\vec{s}_1 \otimes \vec{s}_2)_{-q}^{(2)}, \end{aligned} \quad (8)$$

where  $\alpha_{\text{fs}}$  is the fine structure constant. In the second relation, the spin and orbital part are separated, with  $C_q^2(\theta, \phi)$  representing a reduced spherical harmonic operator and  $(\vec{s}_1 \otimes \vec{s}_2)_{-q}^{(2)}$  the second rank tensor operator that couples the spins [26]. We took into account the contribution from  $V^d$  by expanding the bases to include the total orbital angular momentum  $l$  and its projection  $m_l$ :  $|lm_l\rangle$ . We calculated the matrix elements of Eq.(8) in the fully uncoupled basis  $|lm_l; \lambda\rangle$ , where  $\lambda$  stands for set of quantum numbers  $\{s_1, m_{s_1}, i_1, m_{i_1}, s_2, m_{s_2}, i_2, m_{i_2}\}$ . With this basis,  $\langle \lambda | V^d | \lambda' \rangle$  takes the simple form [27]

$$\delta_{\lambda\lambda'} = (-1)^{-m_l} \frac{\sqrt{6}\alpha_{\text{fs}}^2}{R^3} \sqrt{(2l+1)(2l'+1)}$$

$$\begin{aligned} &\times \begin{pmatrix} l & 2 & l' \\ 0 & 0 & 0 \end{pmatrix} \sum_{q=-2}^2 (-1)^q \begin{pmatrix} l & 2 & l' \\ -m_l & -q & -m_l' \end{pmatrix} \\ &\times \langle s_1 m_{s_1} | \langle s_2 m_{s_2} | [\vec{s}_1 \otimes \vec{s}_2]_q^{(2)} | s_1 m_{s_1}' \rangle | s_2 m_{s_2}' \rangle. \end{aligned} \quad (9)$$

Non-zero matrix elements for  $\Delta l = 0, \pm 2$  and  $l = l' \neq 0$  couple  $s$  and  $d$  waves. We included small corrections to the energies from higher partial waves up to  $l = 4$ .

We have also checked that there are no higher partial wave resonances (*e.g.*,  $p$ -wave,  $l = l' = 1$ ) for the channel [11]. Since the system remains invariant under rotations with respect to the axis of magnetic field, the projection of the total magnetic quantum number  $M_F = m_1 + m_2$  is conserved, and it determines the number of coupled channels. The Feshbach resonances listed in this work are all  $s$ -wave resonances ( $l = 0$ ).

We solve Eq.(6) for different values of magnetic field using the multichannel log-derivative method [28] to obtain the  $\mathbf{S}$ -matrix, from which we extract the radial wave function phase shift  $\eta(k)$  of the initial entrance channel, as well as the scattering length  $a$  using [29]

$$\lim_{k \rightarrow 0} k \cot \eta(k) = -\frac{1}{a}. \quad (10)$$

Here,  $k = \sqrt{2\mu E}/\hbar$  is the wave number associated with the pair of colliding atoms of relative energy  $E$ .

We first calculated the positions of Feshbach resonances for the least energetic hyperfine state  $|\alpha\beta\rangle = |11\rangle$  of  ${}^6\text{Li}+{}^{23}\text{Na}$ . There is no inelastic spin relaxation for this channel which makes it attractive for trapping since the only possible decay channel is through 3-body interactions. Stan *et al.* [11] have measured the positions of three resonances for this state and we used their results to calibrate the singlet and triplet potentials. For each curve, we varied the inner wall by shifting the positions of the data points for separations less than the equilibrium separation  $R_e$  according to  $R_{\text{shifted}} = R + s(R - R_e)/(R_c - R_e)$ , where  $s$  corresponds to the shift of the zero-energy classical turning point  $R_c$ . The best agreement with [11] was obtained with  $s = 0.06170$  a.u. (singlet) and  $s = -0.32878$  a.u. (triplet). It may also be worth noting that we obtained a very good agreement with experimental results only after we included the coupling with nuclear spin and magnetic dipole-dipole interaction. Neglecting these second order terms resulted in agreement up to  $\pm 5$  Gauss for the measured resonances. Our results for the entrance channel [11] and the magnetic field up to 2000 Gauss are shown in Fig. 1 and summarized in Table I. Note that four additional Feshbach resonances were found at higher values of magnetic field, at 1097, 1186, 1766 and 1850 Gauss.

With this set of accurately adjusted potentials, we have also determined the singlet ( $a_S$ ) and triplet ( $a_T$ ) scattering lengths and the energy of the last vibrational level ( $E_{\text{last}}^{S,T}$ ) for both  ${}^6\text{Li}+{}^{23}\text{Na}$  and  ${}^7\text{Li}+{}^{23}\text{Na}$  mixtures (see Table II). Stan *et al.* [11] report a good thermal-

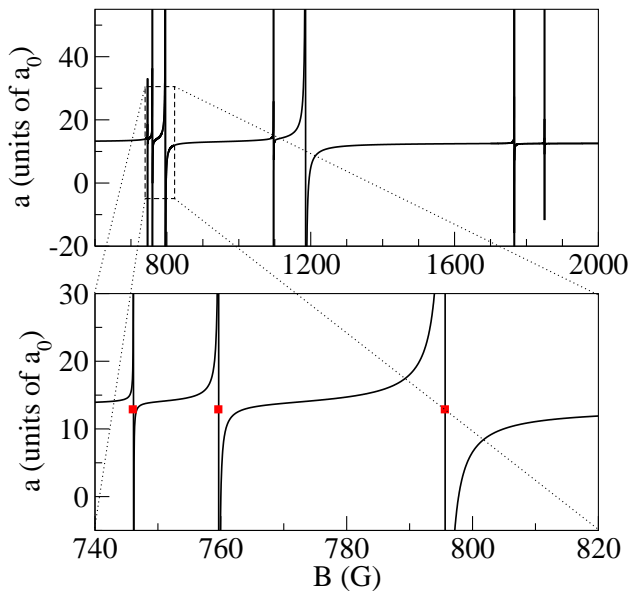


FIG. 1: *Top*: Scattering length for  ${}^6\text{Li}+{}^{23}\text{Na}$  in the entrance channel [11]. Positions and widths of the resonances are given in Table I. *Bottom*: Zoom on the first three resonances. Squares are the experimental positions reported in [11].

TABLE I:  ${}^6\text{Li}+{}^{23}\text{Na}$  - calculated Feshbach resonances ( $l = 0$ ) for the entrance channel [11] and  $B$  up to 2000 Gauss. We compare with the measured position [11], and list the width  $\Delta$  and the background scattering length  $a_{\text{bg}}$ . Both  $a_{\text{bg}}$  and  $\Delta$  were obtained by fitting to  $a_0 = a_{\text{bg}} \left(1 - \frac{\Delta}{B - B_0}\right)$ . Partial waves  $l = 0 \dots 4$  were included in the calculation.

$B_0^{\text{th}}$ (G)	$B_0^{\text{exp}}$ (G) [11]	$\Delta$ (G)	$a_{\text{bg}}$ ( $a_0$ )
746.13	$746.0 \pm 0.4$	0.044	14.003
759.69	$759.6 \pm 0.2$	0.310	13.864
795.61	$795.6 \pm 0.2$	2.177	13.002
1096.68		0.153	13.902
1185.70		8.726	12.673
1766.13		0.156	12.500
1850.13		0.019	12.499

ization rate between for the  ${}^6\text{Li}+{}^{23}\text{Na}$  mixture and exploit the effect for efficient sympathetic cooling. Our results are in agreement with the estimate based on those rates. From the thermalization rate in their experiment, the MIT group estimated the ratio of pure triplet elastic collision between Na-Na ( $\sigma_{AA}$ ) and Li-Na ( $\sigma_{AB}$ ) to be  $\sigma_{AA}/\sigma_{AB} \sim 100$  [30], where  $\sigma_{AA} = 8\pi a_{\text{Na-Na}}^2$  and  $\sigma_{AB} = 4\pi a_{\text{Li-Na}}^2$ , with  $a_{\text{Na-Na}} = 85 a_0$  for the triplet scattering length of Na, one then estimates  $|a_{\text{Li-Na}}| = 12 a_0$  for the triplet case. This estimate is also in agreement with the value of  $|a_T| \approx 15 a_0$  obtained assuming a thermalization time  $\tau_{\text{tot}} \sim 4\tau \sim 15$  sec., where the relationship between  $\tau$  and  $a$  is given in [31]. The uncertainty in the scattering length was determined by adjusting the inner wall of the potentials to match the uncertainty of the resonances (Table I). Alternatively,

TABLE II:  ${}^6,{}^7\text{Li}+{}^{23}\text{Na}$  singlet ( $S$ ) and triplet ( $T$ ) scattering lengths in units of  $a_0$ , the last vibrational level, and the corresponding binding energy. See the text for the description of the uncertainty.

	Present work		Ref. [31]
	${}^7\text{Li}+{}^{23}\text{Na}$	${}^6\text{Li}+{}^{23}\text{Na}$	${}^6\text{Li}+{}^{23}\text{Na}$
$a_S$	$39.7 \pm 0.5$ (1.6)	$15.9 \pm 0.3$ (1.5)	39.2
$a_T$	$36.1 \pm 0.3$ (4.6)	$12.9 \pm 0.6$ (4.5)	31.1
$v_{\text{last}}^S$	47	45	
$v_{\text{last}}^T$	12	11	
$E_{\text{last}}^S$ (MHz)	$-1505 \pm 3$	$-1.6 \pm 0.2$	
$E_{\text{last}}^T$ (MHz)	$-7112 \pm 12$	$-5720 \pm 16$	

we shifted the triplet potential below the last bound state by  $\pm 140$  MHz [11], and then adjusted the inner wall of both singlet and triplet curves to match the experimental position of the resonances. The last triplet bound level was then found with smaller uncertainty to be  $E_{\text{last}}^T = -5720 \pm 16$  MHz, as compared to the estimated value of  $E_{\text{last}}^T = -5550 \pm 140$  MHz of Stan *et al.* [11]. The same procedure was repeated after varying  $C_6$  coefficient by  $\pm 5\%$ , and the results were within the uncertainties given in Table II. Note that Feshbach resonances are very sensitive to the energy of the last vibrational level, which thus can be determined very precisely, while the total number of levels can only be estimated since it depends on the whole potential, which is usually not known accurately enough. For our adjusted triplet state of  ${}^6\text{Li}+{}^{23}\text{Na}$ , we found 11 vibrational levels (see Table II).

Using our adjusted singlet and triplet potential curves, we performed a similar calculation for all entrance channels for  ${}^6\text{Li}+{}^{23}\text{Na}$  and  ${}^7\text{Li}+{}^{23}\text{Na}$ . Predicted positions of Feshbach resonances are shown schematically in Figures 2 and 3. It appears that the  ${}^7\text{Li}+{}^{23}\text{Na}$  mixture has several experimentally attainable Feshbach resonances for the high-field seeking hyperfine states. Altogether, the richness of the scattering properties makes  ${}^6,{}^7\text{Li}+{}^{23}\text{Na}$  mixtures interesting for further exploration.

In conclusion, we present an extensive study of scattering properties in ultracold  ${}^6\text{Li}+{}^{23}\text{Na}$  and  ${}^7\text{Li}+{}^{23}\text{Na}$  mixtures. A full quantum coupled-channel calculation was performed in the field dressed approach, to determine the positions and widths of several Feshbach resonances associated with different entrance channels. The accuracy of our singlet and triplet potentials improved by previous experimental measurements allowed us to very accurately determine the singlet and triplet scattering length of the system, as well as to give an estimated number of vibrational levels in those potentials together with the energy of the last level.

Z. Pavlovic is gratefully acknowledged for providing the original log-derivative program. The authors are grateful to O. Dulieu and M. Aymar for providing us the LiNa *ab initio* potentials, and W. Ketterle and V.

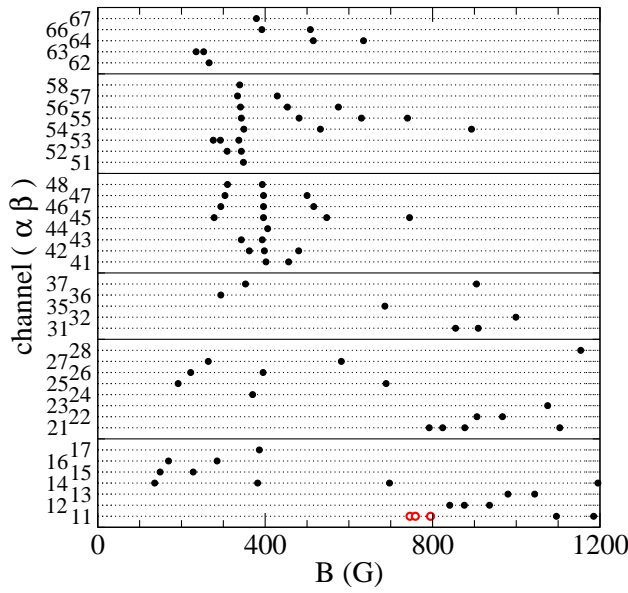


FIG. 2: Feshbach resonances in  ${}^6\text{Li}+{}^{23}\text{Na}$  for different collisional entrance channels. Only channels for which the resonances were found are shown. Open circles for channel |11) were observed experimentally.

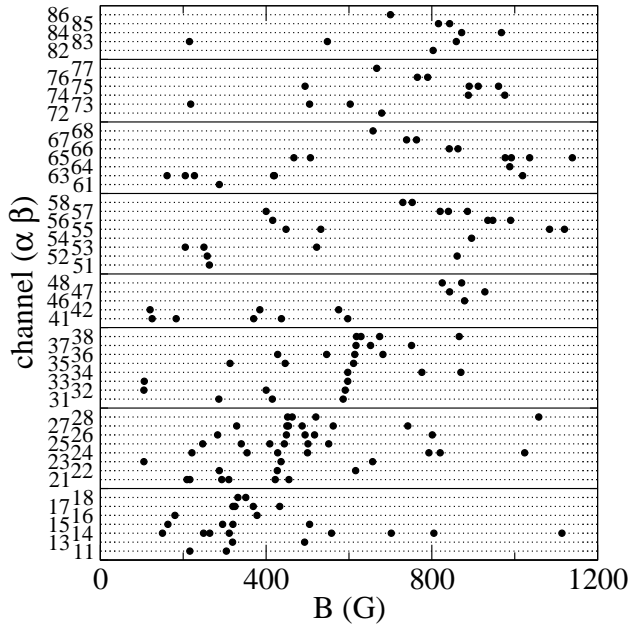


FIG. 3: Same as Fig. 2 for  ${}^7\text{Li}+{}^{23}\text{Na}$ .

Kharchenko for useful discussions. This research was supported by the National Science Foundation.

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